

Towards 100,000 CPU Cycle-Scavenging by Genetic Algorithms

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Abstract

Cycle scavenging systems offer 100s to 100,000s of otherwise-idle CPUs for embarrassingly parallel computations such as genetic algorithms. While genetic algorithms are generally easy to parallelize, cycle scavenged resources come and go at random so some sophistication is necessary, particularly when hundreds of thousands of CPUs are available.

In this paper we propose a master-slave architecture for multi-objective genetic algorithms on cycle scavengers. The architecture consists of slave computations running on computational nodes with relatively small populations, and a central master managing a large pareto front in a disc-based relational data base. Each slave runs an individual genetic algorithm and different slaves use different techniques, evolution-parameters and/or a subset of the objective functions as determined by the master. The slaves accept immigrants from the master and, after evolution, the best individuals emigrate back to the master. Slaves may then get new immigrants and/or evolution policy to be applied to the existing population. Allowing slaves to use different evolution techniques and parameters can, when many CPUs are available, avoid committing to a single evolution concept for a given problem. A sophisticated master can treat the running slaves as a population of evolutionary techniques and parameters that can be evolved.

We examine a web-centric design using standard tools such as web servers, web browsers, PHP, and MySQL. We also consider the applicability of Information Power Grid tools such as the Globus (no relation to the author) Toolkit. We intend to implement this architecture with JavaGenes running on at least two cycle-scavengers: Condor and United Devices. JavaGenes, a genetic algorithm code written in Java, will be used to evolve multi-species reactive molecular force field parameters.

Introduction

NASA has applied genetic algorithms (GAs) to a number of problems. Examples include, but are not limited to, rocket engine design [Akira and Meng-Sing 2001], wing design [Holst and Pulliam 2001], planet discovery [Laughlin and Chambers 2001], circuit design [Lohn and Colombano 1998], molecular design [Globus, et. al. 1999] and molecular force field parameters discovery [Globus, et. al. 2001]. GAs are stochastic, embarrassingly parallel, and can tolerate failures. Thus, GAs are well suited to cycle scavenging computational environments where computers purchased for interactive use also run batch jobs nights, weekends, and at other idle times.

The best-known cycle scavenging computation is seti@home [<http://setiathome.ssl.berkeley.edu/>], currently the largest computation on the planet. Seti@home was using >3 million computers to achieve 23.37 sustained teraflops/sec (979 lifetime teraflops) as of September 2001 [<http://setiathome.ssl.berkeley.edu/totals.html>]. The NASA Advanced Supercomputing Division (NAS [<http://www.nas.nasa.gov>]) has run genetic algorithms using the Condor [<http://www.cs.wisc.edu/condor>] cycle scavenger running on ~350 Sun and SGI workstations. In addition, NAS intends to use the United Devices [<http://www.uniteddevices.com/home.htm>] to run genetic algorithms and other codes on the United Devices MetaProcessor, which cycle scavenges volunteer PCs connected to the Internet. As of September 2001, the MetaProcessor ran on about 900,000 machines [<http://members.ud.com/stats/>]. Entropia [<http://www.entropia.com>] and Parabon [<http://www.parabon.com>] provide services similar to United Devices.

This paper explores some of the issues that must be faced when moving JavaGenes [Globus, et. al. 1999], a genetic algorithm written in Java, from a few hundred processors on the NAS Condor pool to tens of thousands of processors on the United Devices MetaProcessor. There are alternatives to the UD MetaProcessor, but United Devices is interested in providing their resources to NASA free of charge.

First, we briefly review the underlying technologies: genetic algorithms and cycle-scavenging.

Genetic Algorithms

Genetic algorithms seek to mimic natural evolution's ability to produce highly functional objects. Natural evolution produces organisms. GAs produce sets of parameters, programs, molecular designs, and many other structures. Genetic algorithms usually solve problems by:

1. Expressing the solution to a problem in a data structure.
2. Randomly generating a population of individual solutions.
3. Repeatedly selecting parent individuals at random with a bias towards better individuals and applying transmission operators to produce children. Transmission operators include:
 1. Crossover: each of two parents is divided into two parts and one part from each parent is combined into a child.
 2. Mutation: a single "parent" is randomly modified to generate a child.
4. Continuing until an acceptable solution is found or exhaustion sets in.

Better individuals are determined by a "fitness function." Single objective fitness functions produce a number (the "fitness") that can be compared to determine the better individual. Multi-objective fitness functions produce multiple fitness values for each individual, and comparing two individuals is more complex since each individual may be superior in different objectives. For example, one wing design may have low drag but low lift as well, while a second wing may have high drag but have very high lift. One cannot trivially say which wing is better. For multi-objective GAs, one attempts to find the "pareto front," a set of individuals where, for each individual in the front no other individual is superior in every objective.

For most GAs, fitness function evaluation is by far the most time consuming step, and each fitness evaluation is typically completely independent. This means that the main loop is embarrassingly parallel (except for insertion and removal from the population). Also, since GAs are stochastic, a single run rarely tells you much. Just as biologists must conduct experiments with large numbers of animals, GA practitioners often run many copies of the same code with the same inputs (except the random number seed) to get statistically reliable results. Note that if enough copies are run, it is acceptable to lose some runs to system crashes, machines being turned off, or whatever.

Cycle-Scavenging

Cycle-scavenging systems typically use machines purchased for other purposes to run batch jobs at night, weekends, and other idle times. Cycle-scavenging systems typically gain and lose machines at unpredictable times as interactive users start or stop using their machines, new machines are purchased, machines are removed from the network, etc. Most cycle-scavengers will move jobs from machine to machine as necessary

Condor

Condor [Litzkow, et al. 1988] utilizes a cluster of UNIX and Windows NT workstations on a network. The NAS Condor pool consists of approximately 350 SGI and Sun workstations purchased and used for software development, visualization, email, document preparation, etc. Each workstation runs a daemon that watches user IO and CPU load. When a workstation has been idle for 2 hours, a job from the batch queue is assigned to the workstation and will run until the daemon detects a keystroke, mouse motion, or high non-Condor CPU usage. At that point, the job will be removed from the workstation and placed back on the batch queue.

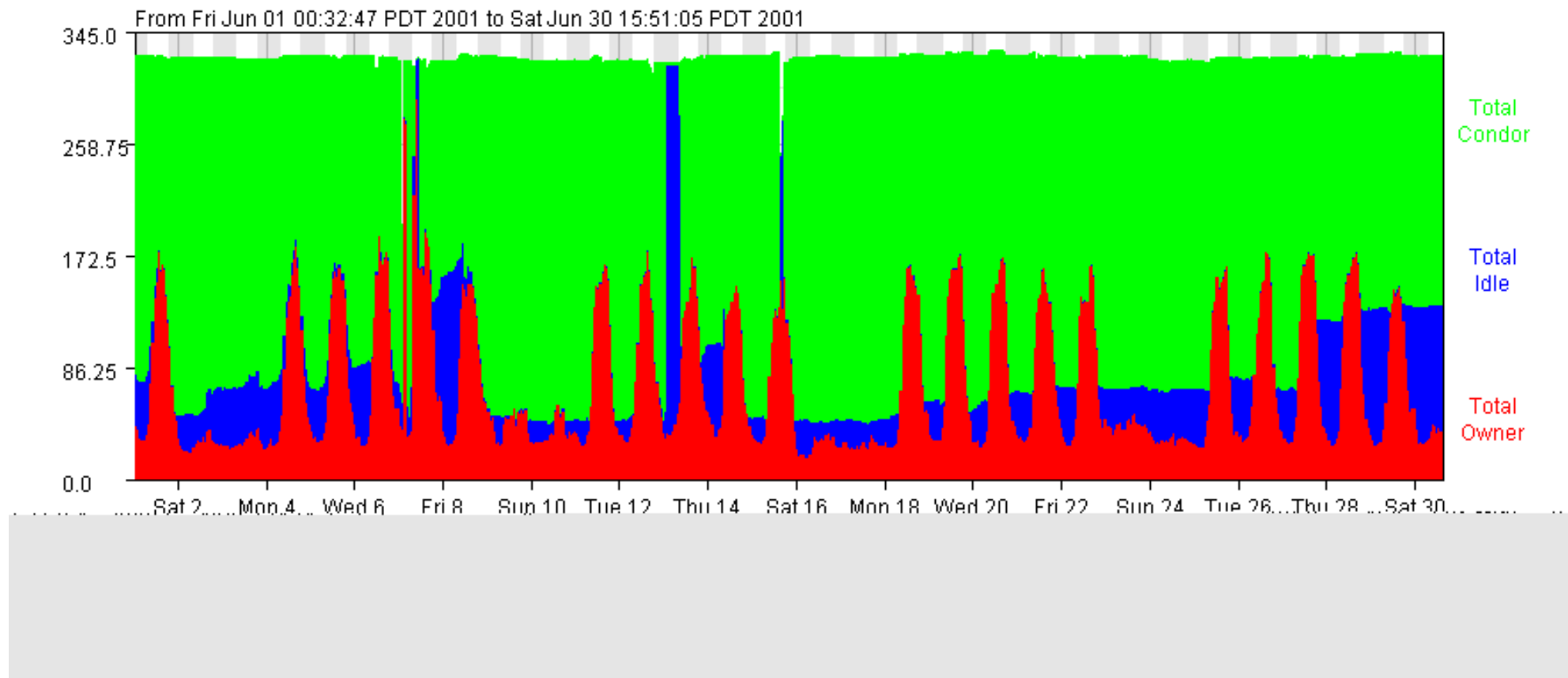


Figure 1: NAS workstation usage for June 2001. Note the regular patterns of five red peaks when workstations are in use during normal business hours. The green represents Condor enabled batch computation. Only the relatively small amount of blue indicates wasted CPU cycles. The tall blue spikes are upgrade times when Condor calculations were temporarily suspended.

Since Condor runs on collections of workstations continuously connected to a network, IO to and from each job can run in the hundreds of megabytes or even a few gigabytes for long running jobs. However, communication between jobs is difficult since jobs are always starting and stopping. Condor has a mechanism to set up master-slave messaging relationships via PVM [Goux, et. al 2000], but JavaGenes does not use it. MPI is not used since MPI 1 does not allow processes to be added or subtracted from an application.

United Devices

United Devices is one of several companies exploiting the success of seti@home by developing systems to cycle-scamge PCs. Motivated by a project to screen potential cancer drugs, people around the world have volunteered approximately 900,000 PCs to the United Devices MetaProcessor. The drug screening runs in background and limits it's memory, disc and CPU usage. United Devices has signed a Letter of Intent with the NAS to execute NASA codes on the MetaProcessor at no cost and a Space Act Agreement is under negotiation. NASA plans to port JavaGenes and other applications to the MetaProcessor. For JavaGenes, this will require major changes to take advantage of the much larger number of processors and accommodate slower network connections. The MetaProcessor is designed for intermittently connected 56Kbaud modems, although perhaps 80% of the PCs in the MetaProcessor are continuously connected by broadband (DSL, cable modem, T1 lines, etc.).

JavaGenes: Current Status

The JavaGenes project presently runs a genetic algorithm on the NAS Condor Pool [Globus, et. al. 2000b]. JavaGenes is currently a single objective GA written in Java which evolves parameters for molecular force fields, molecules, and digital circuits. For the purposes of this paper, we will only consider evolving molecular force field parameters. Molecular force fields are potential functions that calculate the energy of molecules and/or molecular complexes. The reactive, multi-species potentials of interest have ~5-50 parameters for two species; thus, JavaGenes individuals consist of 5-50 floating point numbers. The fitness is the root-mean-square of the difference of externally calculated energies for a set of molecules and energies calculated using the parameters of a given individual. External energies can be calculated by expensive, high-quality quantum codes.

As the best approach to evolving molecular force field parameters is unknown, JavaGenes is used to conduct experiments in genetic algorithm techniques and genetic-algorithm-parameters for the search. Most experiments involve 30-50 jobs using the same GA-parameters (except the random number seed), which means 90-150 jobs for an experiment involving three conditions. Individual jobs run from a few hours to a few weeks. Checkpointing is implemented by JavaGenes and all IO uses the NFS automounter to place results on a single workstation. Analysis of results is via perl scripts run under cron late at night. The scripts generate html files with links to gif files of two dimensional plots. A typical display consists of one plot for each parameter being evolved. Each plot is the value of the best individual (vertical axis) vs generation (horizontal axis). Colors indicate different jobs. Parts of the output are moved to an externally accessible web server so that analysis can be location independent.

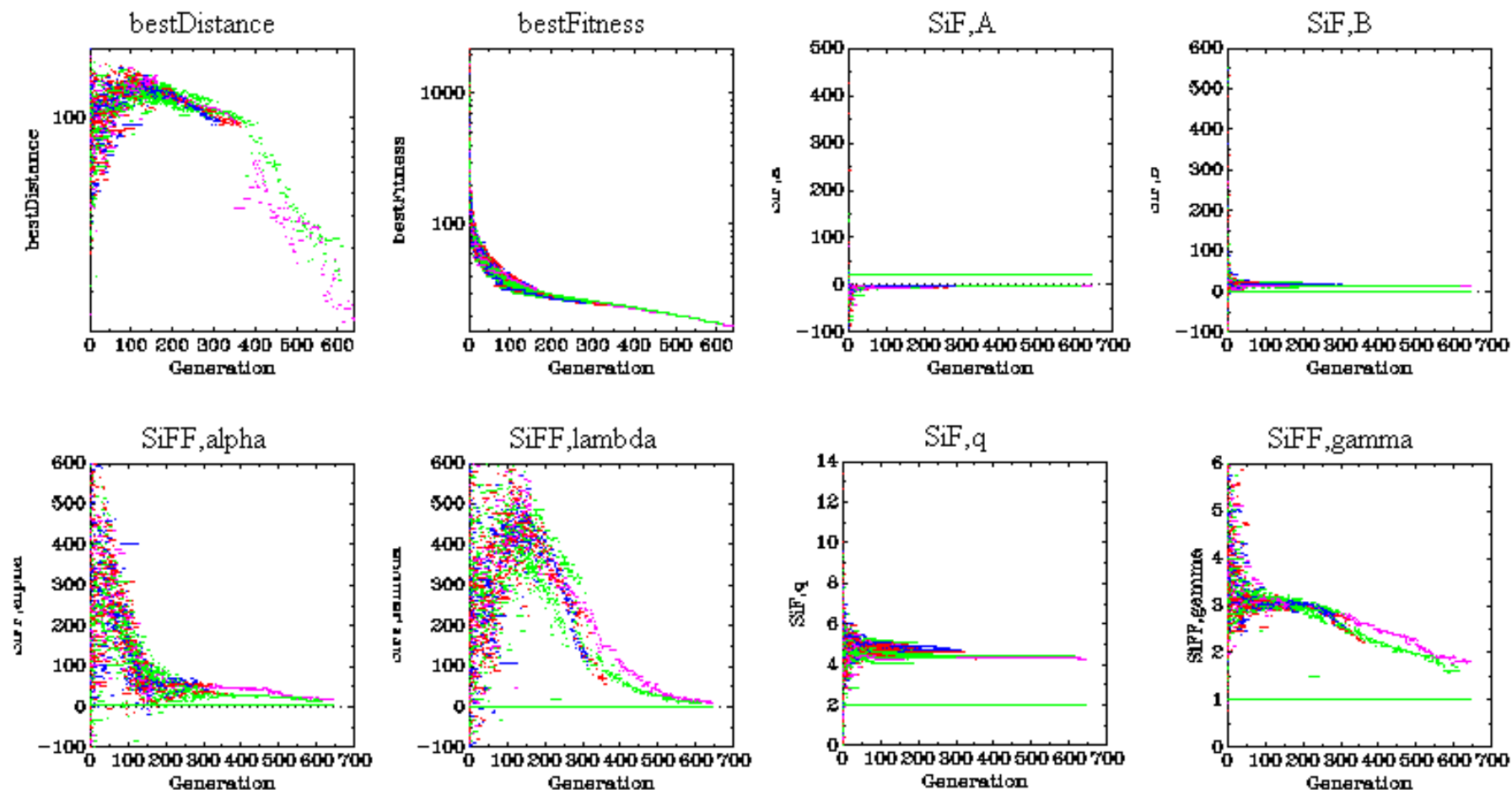


Figure 2: Molecular force field fitness and parameters evolving over time.

Recently, JavaGenes has been modified to pass individuals from one job into the starting population of another job. This allows a run that generates, say, Si (silicon) parameters to provide a starting point that evolves Si and F parameters. However, immigration is accomplished basically by hand: perl scripts remove the best individual from a job's output files and format an input file for another job. The second job reads the input file and modifies the starting population by putting in some number of immigrants. The second job can alternately use the immigrant to determine, for all time, some of the parameters. This technique is useful when the Si parameters have been accurately evolved and can then be used to evolve Si-F parameters.

New Design

We examine the objectives and criteria for the design. After a brief discussion of our approach to multi-objective GAs for this project, we examine a web-centric design based on current standard software and the status of IPG software with regard to cycle-scavenged computation.

Objectives

The JavaGenes design described below is intended to:

- Run on both Condor and the UD MetaProcessor with few or no source code changes and allow for future ports to other platforms (e.g., Entropia and Parabon).
- Take advantage of up to 100,000 processors. It is unlikely that the full MetaProcessor will be available for NASA jobs, so the 100,000 target is probably more than adequate.
- Accommodate broadband connected machines only. Machines in the NAS Condor pool have continuous connectivity to a fast LAN. Approximately 80% of the UD MetaProcessor compute nodes are broadband connected so it doesn't make sense to design for 56Kbaud modems..

Criteria

The design should be judged according to the following special criteria (plus the usual motherhoods):

- Make appropriate use of cycle-scavenged computational nodes. Since compute nodes are very plentiful on the MetaProcessor, substantial inefficiencies may be tolerated to achieve other goals.
- Tolerate substantial random loss of computational nodes. Compute nodes on Condor and the MetaProcessor are constantly being turned-off, removed from the system, etc.
- Tolerate loss of network connectivity. While we are restricting ourselves to broadband connectivity, network connectivity can still be lost for a variety of reasons and this should not be fatal to the computation.
- Tolerate occasional loss of central facilities. Any central facility will fail occasionally and this should not fatally affect the computation.
- Use a multi-objective GA to take advantage of experimental data. The single objective GA has problems getting the right answers. It is believed that this can be improved by incorporating experimental data into the fitness function. It appears that the best way to do this is to use a multiple objective GA.
- Require little or no GA parameter/policy tweaking. The bane of GA research is the large numbers of GA-parameters (e.g., population size, mutation frequency, etc.) and techniques that must be searched to find the "right" approach. On the MetaProcessor, we intend to experiment with evolving the GA-parameter settings while simultaneously searching for the solution.
- Have security sufficient to run slaves on any machine on the internet. Anyone on the internet can volunteer their PC to the UD MetaProcessor. Thus, a variety of security risks must be addressed.

Multi-Objective Approach

JavaGenes molecular force field parameter evolution is expected to have 5-10 objectives. The pareto front in a such a higher dimensional space is huge and requires many points to sample effectively. However, the number of immigrants that may be sent from one slave is limited by bandwidth and master

processing power. Therefor, a multi-objective fitness function for the slaves that identifies one or a few 'best' individuals is desirable, while a large pareto front of individuals can be managed by the master on disc.

A multi-objective GA that identifies a few best individuals has been developed at Ames [Lohn, et. al. 2000]. In this system, a population of teachers evolve in parallel with the main population. Each teacher consists of a desired level of performance for each objective. The fitness of a teacher is inversely proportional to the number of individuals that passes the teacher's test for all objectives -- or the worst possible fitness if no individual can pass the teacher's test. The fitness of each individual is proportional to the number of teacher-tests the individual passes. As evolution progresses, the teacher tests become more difficult and the population improves, but there is always one or a few individuals with the highest fitness. These will be chosen for emigration.

Web-Centric Design

Components

We propose a master-slave architecture with immigrants passing from slave to slave through the master. Communication is via a web server with a relational database backend.

The design consists of seven elements: master, slave, web server, database server, cycle scavenger, web browser, and charting applet. Figure 3 shows their relationships:

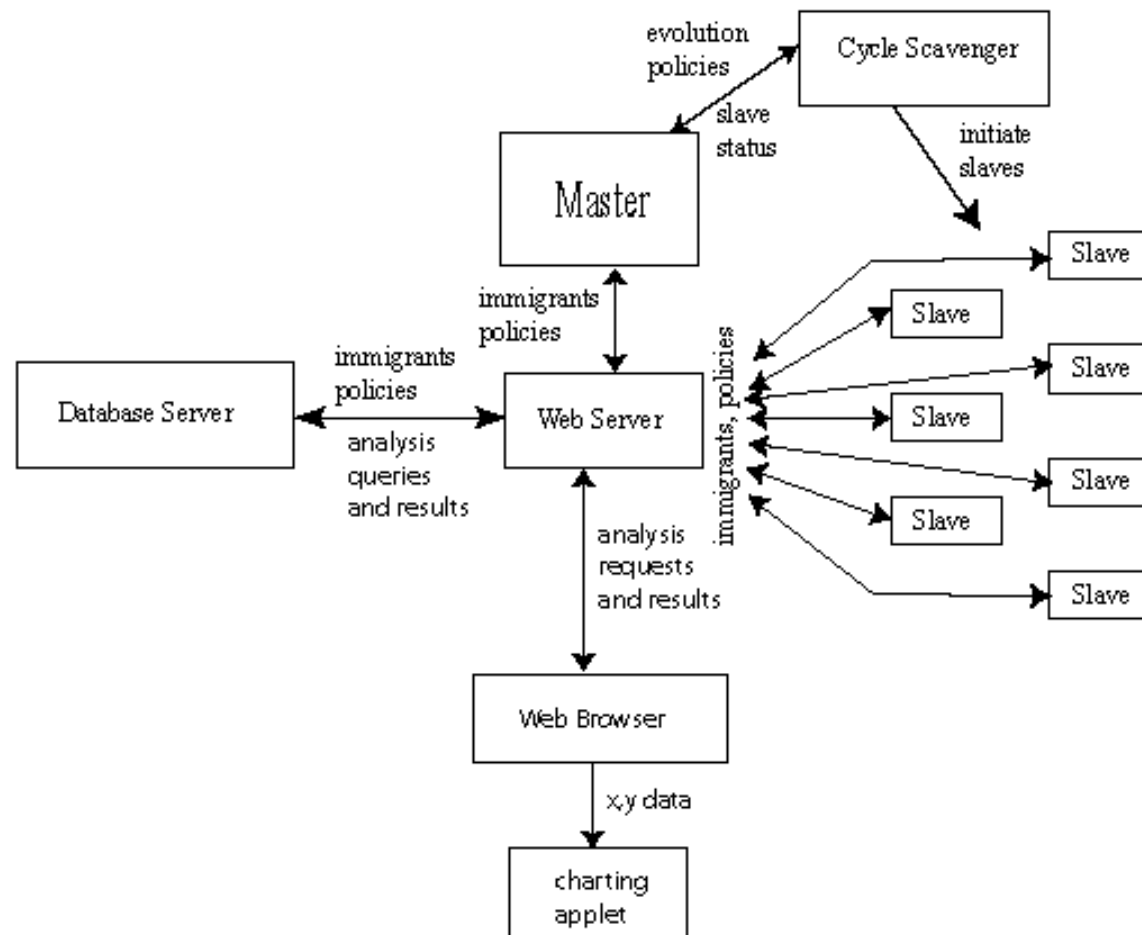


Figure 3: planned web-centric JavaGenes architecture.

1. Slaves: slaves manage a population. Slaves run a multi-objective GA until killed. The GA uses [Lohn, et. al. 2000]'s technique where an evolving population of teachers can be used to determine a few best individuals. Periodically, slaves send the best individuals to the web server, check for immigrants, and check for a new policy. Each of these may be at different time intervals. If a new policy is provided, the current best individual is sent to the database so improvement can be measured.
2. Master: manages a central database of individuals consisting of the current pareto front and it's history. The master also determines where immigrants go and the evolution policy of the slaves. The evolution/immigration policies can evolve as the computation proceeds. A policy's fitness is the fitness of the best individual the slave has produced and the improvement of the best individual since the last policy change. The evolution policy includes:

- Population size
 - Transmission operators, their parameters, and frequency of use
 - Method for choosing parents
 - Subset of objective to evolve
 - Immigrant and emigrant frequency
 - Frequency of policy change
 - etc.
3. Database server: off-the-shelf database server holding the pareto front and it's history. The baseline design uses mySQL [<http://www.mysql.com>].
 4. Web Server: off-the-shelf web sever. Except for initiation and termination, all slave communication passes through the web server using SSL. PHP pages implement the interaction. All access to the database must pass through the web server. This architecture means that the slaves need no special IO facilities on their hosts (other than internet access and standard Java libraries). In particular, after initiation all IO is Cycle Scavenger independent.
 5. Cycle Scavenger: off-the-shelf cycle scavenger (Condor, United Devices, Entropia, Parabon, etc.). This element initiates, terminates and manages the slave processes.
 6. Web Browser: off-the-shelf web browser. This is used for requesting data analysis (via SQL queries) and examining results.
 7. Charting applet: modified off-the-shelf applet. This applet draws small multiples (see figure 2) of two dimensional charts of the data returned by SQL queries.

Performance

Large numbers of slaves have the potential to overwhelm the master, web server, and/or database server with requests and information. For this reason, every slave interaction with the web server will receive a time in milliseconds as a response. This time is the minimum time before the slave may re-contact the web server. By observing the load on the central systems and changing this time value, the master can keep the load on the central systems at reasonable levels. Also, rogue slaves may be detected if they re-contact the web-server before the requested time.

Security

It will be possible for sophisticated individuals to feed bogus data to JavaGenes. This must be detected and ignored. Also, it may be possible to reverse engineer the JavaGenes slave code from the Java byte code sent to the slaves. JavaGenes is well documented in the open literature and may be distributed within the US, so while steps to prevent this problem should be taken, absolute assurance is overkill. Finally, unauthorized individuals may try to gather information on the computation by examining IO. Since each slave sees only a tiny fraction of the computation, and the results of the calculation are expected to be published in the open literature, this problem also does not require iron-clad security.

There are a couple of possible attacks on proposed system:

- An unauthorized party could take control of the code and/or data sent to a slave. However, the Condor nodes are inside the NAS security walls and United Devices encrypts all data sent to computational nodes. Therefor, these data are only accessible in memory. Furthermore, Java byte code can be obscured to make reverse engineering of the byte code difficult.
- An unauthorized party could modify slaves to send incorrect data to the master. The only possible truly wrong data is the fitness values for the immigrants. However, the number of immigrants is tiny compared to the total population under evolution (a ratio of perhaps 1/100,000 or greater). Therefor, the master can simply re-evaluate the fitness (in this case independent of the teachers). Also, immigrants can be sent via SSL to make

reverse engineering the format difficult.

- An unauthorized party could flood the master with messages in a denial-of-service attack. The timing approach mentioned above can limit this, although any web server is subject to such an attack.
- An unauthorized party could attempt to corrupt the database directly, without going through the web server. Currently, the NAS MySQL server only allows access from build-dev.nas.nasa.gov. Furthermore, MySQL database privileges may be set to minimize the capabilities of each part of the system. Namely:
 - Slaves may only add and retrieve from/to the immigrant tables and retrieve from policy tables
 - Master may only retrieve/delete from immigrant tables, add to history tables, add/delete/retrieve from policy tables, create databases and tables.
 - Analysis may only retrieve data.

Security is also an issue for the proposed analysis capabilities. While unauthorized reading of the data is of relatively little concern, since it will be published in the open literature eventually anyway, modification of the database and denial of service attacks could be problematic. These can be addressed by password protecting the relevant web pages and by limiting access to the machines used by the author and his collaborators.

IPG Design

It is possible to implement the design as a message passing system by replacing the web-server with a message passer for the compute portion of the system. The IPG currently provides an implementation of MPI 1.1 [<http://www-unix.mcs.anl.gov/mpi>] called MPICH-G2 [<http://www.niu.edu/mpi>]. However, MPI 1 does not allow processes to be added or removed once an application has started, so MPICH-G2 cannot be used in a cycle-scavenging environment. MPI 2 does allow for dynamic changes to an application's processor so it may work. Although MPICH-G2 implements part of MPI 2, it does not implement a dynamic process pool.

Also, the MPI standard is explicitly intended for C and FORTRAN, not Java, programs, so a JNI (Java Native Interface) is necessary for Java programs to connect to an MPI library. This makes applications somewhat less platform independent since a separate native code library is necessary for each architecture. Nonetheless, if a MPI 2 implementation were available as part of cycle-scavenger compute node implementation one could replace the web server with a central message handler. However, as Java has excellent communication facilities and MPI has a very small market share, it may be difficult to convince commercial vendors to add MPI 2 to their cycle-scavenging communication facilities.

Another approach to using current IPG capabilities would be to use globus-io [http://www.globus.org/v1.1/io/globus_io.html] to pass data to and from a central machine. A polling mechanism could then insert the data into the database using the web server and/or a more direct interface. globus_io provides both security and non-blocking IO. Again, as with MPI, globus-io is intended for C and FORTRAN programmers so a JNI interface would be necessary. Globus-io could be added to the Condor installation and be reliably available to Condor programs, however it may be difficult to convince commercial companies to implement globus-io as they already have their own mechanisms for compute nodes to communicate with their central servers.

In the next few months, it seems impractical to use globus communication libraries for cycle-scavenging applications. However, the cycle-scavenging community seems to be ripe for some kind of standardization, and perhaps the IPG can help. Condor is already moving towards IPG integration with Condor-g; and NAS is planning to make the Condor pool accessible to globus jobs on an experimental basis (there are some security concerns). Entropia has announced they will integrate their product with the IPG [http://www.entropia.com/release_09272001.asp]. As NASA works with the vendors there

should be opportunities to move towards a more integrated set of systems that may even allow applications to take advantage of multiple cycle-scarvers. For the present effort, certain tasks (e.g., immigrant validation) could be performed on trusted Condor nodes while the bulk of evolution continues on untrusted United Devices nodes. The lessons learned should be valuable in developing interoperability standards for cycle-scarvers in the same manner that the IPG is developing interoperability for more conventional supercomputers.

There is one area the IPG could help with in the near future. If both Condor and United Devices were accessible to globus jobs, then the master would see a uniform environment for initiating and terminating jobs. NAS Condor pool accessibility to globus jobs will be tested in the next few months, and it is possible, in principle, to build a globus front end for the United Devices MetaProcessor. Although the details of Entropia/globus integration are not yet known, they almost certainly include running globus jobs on Entropia system. Having all systems implement globus job control would simplify job initiation and management code in the master.

Conclusion

In the next several months JavaGenes is expected to evolve from a simple genetic algorithm with disc IO run on the NAS Condor pool to a web-centric application distributed across the Internet with a relational database for storage using IPG process management. This change is driven by the need to move from execution on a pool of a few hundred UNIX workstations in one location to execution on up to a hundred thousand PCs scattered around the world. This will allow real world experience with massively distributed cycle-scarving applications to drive IPG standardization in this area.

Acknowledgments

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JavaGenes: Evolving Molecular Force Field Parameters

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This is an abstract for a presentation given at the
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There will be a link from here to the full article when it is available on the web.

Accurate molecular dynamics simulation of reactive multi-species systems is important to the design of artificial molecular machines. For example, the existing reactive hydrocarbon Brenner's potential has been used to design gears, hinges, three-way junctions, and bearings and helped motivate the design of a hydrocarbon assembler. Unfortunately, reactive multi-species potentials are only available for C-H-nobel gas, Si-F, Si-C-Ge and a few others. This is not sufficient to design molecular factories of the type envisioned by Drexler. Furthermore, developing reactive multi-species potentials is difficult, time consuming, tedious, failure prone and, thus, rarely attempted.

There are two parts to developing any force field: finding a functional form that reflects the physics and choosing the parameters required by the form. Much of the tedium is in the parameterization. We hypothesize that this step can be automated by large computations on cycle-harvested desktop computers. By automating parameterization, exploration of functional forms should be enhanced.

Given a functional form, the parameters are typically chosen to fit experimental values and/or ab initio calculations. The fitting process can be difficult because functional forms usually have many local minima that tend to trap search algorithms. We are developing the JavaGenes genetic algorithm to evolve force field parameters. Genetic algorithms are somewhat less likely to fall into local minima than

simulated annealing or hill climbing. For proof of concept, we have evolved the (Stillinger and Weber 90) published parameters for Si and F separately with good, although not yet perfect, results. Over the next few months we expect to evolve the full, combined Si-F published parameters and compare the results with parameters fitted to ab initio energy calculations.

Results

Table 1 shows results evolving the (Stillinger and Weber 90) Si parameters: For two body parameters we fit the energies of 100 Si dimers spaced 0.5-3.7 angstroms apart. The three body parameters were evolved separately with the two body parameters fixed to the best values from the two-body run and fit to 400 Si tetrahedra randomized around the low energy conformation.

Table 1

Parameter	Published value	Evolved value
A	7.049556277	7.062138589233899
B	0.6022245584	0.6283594386627
C	1.0	0.9999066666678916
p	4.0	3.9970443831775535
q	0.0	0.005038128110635121
Three body parameters		
alpha	0.0	-0.00476705603392214
lambda	21.0	21.030398353724657
gamma	1.2	1.2003753288365615

Table 2 shows results evolving the (Stillinger and Weber 90) F parameters. For two body parameters we fit the energies of 100 F dimers spaced 0.5-5 angstroms apart. The three body parameters were evolved separately with the two body parameters fixed and fit to 100 F₂+F conformations.

Table 2

Parameter	Published value	Evolved Value
A	0.52276	0.536060720470749
B	0.11277	0.123804003816043856
C	0.579495	0.5794579857222181
p	8.0	7.884508889552029

q	4.0	4.055374744348555
Three body parameters		
alpha	38.295	31.904841586417522
lambda	-19.1475	-23.848659093495885
gamma	1.738485	1.84226440597913
delta	0.0818182	6.711483050303828
m	4.0	2.2224104136309757
beta	0.579495	2.4738447463466304

Note: The functional form was transformed to give all terms an identical form, except FFF where the last three parameters are unique. These three parameters have not yet been accurately evolved by JavaGenes. Once the proof of concept is complete, we will use the procedures developed to create reactive force fields for new systems, e.g., BN nanotubes.

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The Condor® Project Homepage

The goal of the Condor Project is to develop, implement, deploy, and evaluate mechanisms and policies that support [High Throughput Computing \(HTC\)](#) on large collections of distributively owned computing resources. Guided by both the technological and sociological challenges of such a computing environment, the [Condor Team](#) has been building software tools that enable scientists and engineers to increase their computing throughput.

Recent News

(10/01) [Condor Version 6.3.1 for UNIX - support for Redhat 7.1 Linux!](#)

Condor 6.3.1, the second release of our development series is now available. It's available from the [Downloads](#) page. You can read the ChangeLog [in the version history](#) section of the manual.

(9/01) Read about [NMI](#), the NSF Middleware Initiative, a new venture.

(8/01) [Condor Version 6.2.1 for UNIX and NT released!](#)

Condor 6.2.1, the second release of our stable series is now available. It's available from the [Downloads](#) page. You can read the ChangeLog [in the version history](#) section of the manual.

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